# Self-consistent calculations of quadrupole moments of the first $2^+$ states in Sn and Pb isotopes

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A method of calculating static moments of excited states and transitions between excited states is formulated for non-magic nuclei within the Green function formalism. For these characteristics, it leads to a noticeable difference from the standard QRPA approach. Quadrupole moments of the first $2^+$ states in Sn and Pb isotopes are calculated using the self-consistent TFFS based on the Energy Density Functional by Fayans et al. with the set of parameters DF3-a fixed previously. A reasonable agreement with available experimental data is obtained.

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## I. INTRODUCTION

To reliably predict properties of unstable nuclei at the modern level of microscopic nuclear theory at least two conditions need to be fulfilled. First, it is necessary to take into account the single-particle continuum which is especially important for the description of nuclei with small separation energies. Second, an approach should be used with the self-consistency relation between the mean field and effective interaction. This makes it possible to use only one set of parameters instead of two sets, for the effective interaction and mean field, in non-self-consistent approaches. The self-consistency improved noticeably the predictive power of the theory even on the RPA or QRPA level, for the review see [1].

Nowadays, it is also necessary to add to these conditions the accounting for phonon coupling (PC). This problem has been studied for a long time within several approaches which are referred as the Quasiparticle-Phonon model (QPM) [2], (Q)RPA+PC [3], Extended Theory of Finite Fermi Systems (ETFFS) [4] (non-selfconsistent cases) and the self-consistent versions, (Q)RPA+PC [5] and the ETFFS in the Quasiparticle Time Blocking Approximation [6] (ETFFS(QTBA)) [7]. For magic and semi-magic nuclei, such approaches are based on the fact that in these nuclei there is a small parameter $g^2$, the dimensionless square of the phonon creation amplitude. For brevity, we call this weak PC approximation where only the $g^2$ terms are taken into account the $g^2$ approximation.

In the framework of the Green function (GF) formalism, all the conditions under discussion have been realized and have shown their importance for stable nuclei too [4, 6, 7]. However, all the above mentioned approaches dealing with the PC did not take into account *all* the $g^2$ terms, thus limiting themselves with the pole diagrams only, see the first diagram in Fig. 1 where diagrams for the mass operator are displayed. The second diagram represents the sum of all the non-pole diagrams that we call the phonon tadpole now.

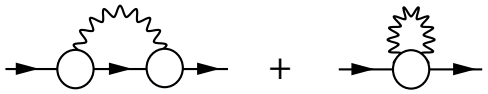

FIG. 1: $g^2$ order corrections to the mass operator in magic nuclei. The circles with one wavy line in the first term are the phonon creation amplitudes. The second term is the phonon tadpole.

The problem of consistent consideration of all the $g^2$ terms including tadpoles was analyzed in the article by Khodel [8] on the base of the general self-consistency relations for finite Fermi systems [9]. The method developed was practically realized for magic nuclei, mainly for static nuclear characteristics, within the self-consistent TFFS [10]. It was found that, as a rule, the tadpole contributions in magic nuclei are noticeable and are often of opposite sign as compared with those of the pole terms. The first attempts to include the tadpole effects for nuclei with pairing and for consideration of dynamical problems were recently made in [11] and [12], respectively.

In the PC problem, the $g^2$ corrections to the mean field shown in Fig.1 have been mainly studied up to now [10]. They are, as a rule, smaller than the corresponding mean field values and could be partially hidden in the phe-

nomenological parameters used. In this work, within the GF method, we concentrate our attention on more delicate characteristics which are proportional to $g^2$ themselves. Namely, we analyze the static moments of excited states and transitions between excited states. To ensure the self-consistency, we use the self-consistent TFFS based on the Energy Density Functional by Fayans et al. [13] with the DF3-a set of parameters fixed previously [14]. We briefly consider some static and low-energy characteristics in magic and generalize the method for non-magic even-even nuclei (Sects. II and III, respectively). Within this approach, and using some approximations we perform the first self-consistent calculations of static moments of the first $2^+$ excited states in even-even tin and lead isotopes (Sect.IV)

The quadrupole moments of excited states have been calculated earlier within QPM in [15, 16]. In Ref.[17], the authors performed the calculations, which are similar to ours in Sect.IV, using the method later called Nuclear Field Theory and a phenomenological approach with the set of phenomenological parameters taken from experiment for each nucleus. In [17], a reasonable agreement was obtained with the experimental data for Sn and Ni isotopes when available at that time. The main difference of our approach from [15–17] is its full self-consistency on the (Q)RPA level and absence of any phenomenological or fitted parameters. These features will allow characteristics of unstable nuclei to be calculated.

## II. MAGIC NUCLEI

To describe the PC effects in magic nuclei with the consistent account of all the $g^2$ terms, we follow the method by Khodel [8]. In the $g^2$ approximation, the matrix element $M_{LL}$ for a static moment of the excited state (phonon) with the orbital angular moments $L$ in a static external field $V^0$, is determined in terms of the change of the one-particle GF in the field of this phonon:

$$M_{LL} = \int V^0(\mathbf{r})\delta^{(2)}_{LL}G(\mathbf{r},\mathbf{r},\varepsilon)d\mathbf{r}\frac{d\varepsilon}{2\pi\imath}, \qquad (1)$$

where

$$\delta^{(2)}_{LL}G = \delta_L(Gg_LG) = G(\varepsilon)g_LG(\varepsilon+\omega_L)g_LG(\varepsilon) \qquad (2)$$
$$+G(\varepsilon)g_LG(\varepsilon-\omega_L)g_LG(\varepsilon) + G(\varepsilon)\delta_Lg_LG(\varepsilon),$$

where $g_L$ is the amplitude for the production of the L phonon with the energy $\omega_L$ and $\delta_Lg_L$, the variation of $g_L$ in the field of other $L$ phonon. Substituting Eq. (2) into Eq. (1), we obtain in the symbolic form:

$$M_{LL} = V^0Gg_LGg_LG + V^0GG\delta_Lg_L, \qquad (3)$$

which is illustrated in Fig.2 where the blocks $g_L$ and $\delta_Lg_L$ enter.

It is convenient to transform this expression in such a way that the effective field $V$ will appear instead of the external field $V^0$. They are connected with the TFFS equation, [18]

$$V = V^0 + \mathcal{F}AV, \qquad (4)$$

where $\mathcal{F}$ is the effective particle-hole (ph) interaction and $A$ is the ph propagator (the integral over energy of the product of two single-particle GF's). After regrouping the terms in Eq.(3) and iterating the integral equation for the quantity $\delta_Lg_L$ in the effective interaction $\mathcal{F}$ (for details, see [10, 12]), we obtain the ultimate expression,

$$M_{LL} = VGg_LGg_LG + VGG\delta_L\mathcal{F}GGg_L, \qquad (5)$$

which is illustrated in Fig. 3. It contains now the effective field $V$, instead of $V^0$ in Eq. 3, and the quantity $\delta_L\mathcal{F}$ in the second term which denotes the variation of the effective ph interaction $\mathcal{F}$ in the field of the $L$ phonon. For the density dependent TFFS effective interaction $\mathcal{F}(\rho)$, the following ansatz can be readily obtained [8, 10]:

$$\delta_L\mathcal{F}(\mathbf{r}) = \frac{\partial\mathcal{F}}{\partial\rho}\rho^{\rm tr}_L(r)Y_{LM}(\mathbf{n}), \qquad (6)$$

where $\rho^{\rm tr}_L = Ag_L$ is the transition density for the $L$ phonon excitation. The first term of Eq.(5) coincides with the result by Speth [19] while the second one with the $\delta_L\mathcal{F}$ quantity is a generalization to take into account all the $g^2$ terms.

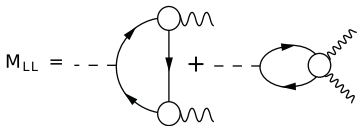


FIG. 2: Matrix element $M_{LL}$ for magic nuclei, Eq. (3).

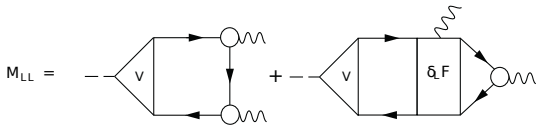


FIG. 3: Matrix element $M_{LL}$ in the form of Eq. (5).

All the above equations can be readily modified for such processes as the transition between the excited states $L$ and $L'$ in the external field $V^0(\omega = \omega_{L'} - \omega_L)$ or the excitation of the two-phonon state $L + L'$ in the external field $V^0(\omega = \omega_{L'} + \omega_L)$. The static moments case corresponds to $\omega = 0$.

## III. NON-MAGIC NUCLEI. COMPARISON WITH QRPA.

In the case of nuclei with pairing, it is necessary to use four GF's ($G, G^h, F^{(1)}, F^{(2)}$ in the usual notation [18]). To describe phonons, one has to use the complete set of

the QRPA equations which include the ph, hp, pp, and hh channels and four effective fields $V$, $V^h$, $d^{(1)}$ and $d^{(2)}$ [18], respectively. As the pp and hh channels give a small contribution in the case of the first $2^+$ levels [20], which is considered in the next Section, we do not consider these channels and, accordingly, the fields $d^{(1)}$ and $d^{(2)}$. Then we obtain eight terms $M^{(i)}_{LL'}$ instead of one in Eq.(5). The typical two terms , $M^{(1)}$ and $M^{(5)}$ are shown in Fig.4. In this study we will consider the case without the terms with $\delta_L\mathcal{F}$ and $\delta_L\mathcal{F}^\xi$, see Sect.IV

The integral of the three GF's $A^{(1)\rm pair}_{123}$ has the form

$$A^{(1)\rm pair}_{123}(\omega_L,\omega_{L'}) = \int G_1(\varepsilon)G_2(\varepsilon+\omega_L)G_3(\varepsilon+\omega_{L'})\frac{d\varepsilon}{2\pi\imath}$$
$$= \frac{u_1^2u_2^2v_3^2}{(\omega_L+E_{13})(\omega_{L'}+E_{23})} + \frac{v_1^2v_2^2u_3^2}{(\omega_L-E_{13})(\omega_{L'}-E_{23})}$$
$$+\frac{1}{\omega+E_{12}}\left(\frac{u_1^2v_2^2u_3^2}{E_{23}-\omega_{L'}} - \frac{u_1^2v_2^2u_3^2}{E_{13}+\omega_L}\right) \qquad (7)$$
$$+\frac{1}{\omega-E_{12}}\left(\frac{v_1^2u_2^2v_3^2}{E_{23}+\omega_{L'}} - \frac{v_1^2u_2^2u_3^2}{E_{13}-\omega_L}\right),$$

where $E_{12} = E_1 + E_2, E_1 = \sqrt{(\varepsilon_1-\mu)^2+\Delta_1^2}$ and the low index $1 = (n_1, l_1, j_1)$ (spherical nuclei) is the set of single-particle quantum numbers.

In the pairing case there are eight such integrals of three GF's $A^{(i)\rm pair}_{123}$, where $i$ = 1-8. After a long algebra, one can obtain the final formula for the diagonal matrix element $M_{LL}$ with L = L′, which corresponds to the case of static quadrupole moment of the excited L state. Just this case is considered in the next section .

$$M_{LL} = \sum_{123}(-1)^{M_L+1}\begin{pmatrix} I & L & L \\ 0 & L & -L\end{pmatrix}\begin{Bmatrix} I & L & L \\ j_3 & j_2 & j_1\end{Bmatrix}$$
$$\times <1\parallel V\parallel 2><3\parallel g_L\parallel 1><2\parallel g_L\parallel 3>\sum_{i=1}^{8}A^{(i)\rm pair}_{123}, \quad (8)$$

where

$$\sum_{i=1}^{8}A^{(i)\rm pair}_{123}$$
$$= \left(\frac{1}{(\omega_L+E_{13})(\omega_L+E_{23})} + \frac{1}{(\omega_L-E_{13})(\omega_L-E_{23})}\right)$$
$$\times\left[u_1^2u_2^2v_3^2 - v_1^2v_2^2u_3^2 + \frac{\Delta_1\Delta_2}{4E_1E_2}(u_3^2-v_3^2)\right.$$
$$\left. + \frac{\Delta_1\Delta_3}{4E_1E_3}(u_2^2-v_2^2) + \frac{\Delta_2\Delta_3}{4E_2E_3}(u_1^2-v_1^2)\right] + \qquad (9)$$
$$\frac{1}{E_{12}}\left[\frac{2E_{23}(u_1^2u_3^2v_2^2 - v_1^2v_3^2u_2^2)}{E_{23}^2-\omega_L^2} + \frac{2E_{13}(u_2^2u_3^2v_1^2 - v_3^2v_2^2u_1^2)}{E_{13}^2-\omega_L^2}\right.$$
$$-\left(\frac{\Delta_1\Delta_2}{2E_1E_2}(u_3^2-v_3^2) + \frac{\Delta_1\Delta_3}{2E_1E_3}(u_2^2-v_2^2)\right.$$
$$\left.\left. + \frac{\Delta_2\Delta_3}{2E_2E_3}(u_1^2-v_1^2)\right)\left(\frac{E_{13}}{E_{13}^2-\omega_L^2} + \frac{E_{23}}{E_{23}^2-\omega_L^2}\right)\right].$$

Let us compare this expression with the respective result of QRPA approach. Here we mean the usual way which uses the QRPA wave functions for the matrix element between two excited states. In Ref.[21] the expression for the matrix element (the B(E2) quantity, to be exact) has been derived using the bare external field and, like in our case, the QRPA wave functions without the pp and hh-channels. The first square brackets (in the first half of Eq.(9)) coincide completely with the factor $v^-_{12}u^+_{23}u^+_{31}$ in Refs.[2, 21]. Thus, the first half of Eq.(9) corresponds to the expression $v^-_{12}(\psi_{23}\psi_{31}+\phi_{23}\phi_{31})$ in [21] because the phonon amplitudes $\psi$ and $\phi$ contain, by definition, the denominators $(E_{12}-\omega_L)$ and $(E_{12}+\omega_L)$, respectively. Therefore, the second half of Eq.(9) (with the common factor $1/E_{12}$), generalizes the usual QRPA approach. This part of Eq.(9) describes the contribution of the ground state correlations (the so-called graphs going back) to our "triangle" with the integral of three GF's, see Eq. (7). We will calculate the quantitative contribution of such correlations in the next section. The second generalization is the appearance of the effective field V, which depends on the frequency $\omega = \omega_L \pm \omega'_L$ instead of external field $V^0$, which does not depend on the frequency. The terms with $\delta_L\mathcal{F}$ and $\delta_L\mathcal{F}^\xi$ are the third generalization of the QRPA approach

## IV. CALCULATIONS OF STATIC QUADRUPOLE MOMENTS OF THE FIRST $2^+$ STATES IN TIN AND LEAD ISOTOPES

The quadrupole moment of the excited state L is connected with the matrix element $M_{LL}$, Eq. (8) ($I$ = 2, $V(\mathbf{r}) = V(r)Y_{20}(\mathbf{n})$ ), as follows:

$$Q = \sqrt{\frac{16\pi}{5}}M_{LL}. \qquad (10)$$

In the recent work [22], we calculated the static quadrupole moment of the first $3^-$ level in $^{208}$Pb, using only the first term in Eq. (5) (or Fig. 3), and obtained the value $Q_{\rm theor} = -0.26$ b which is in a reasonable agreement with the experimental one, $Q_{\rm exp} = -0.34\pm0.15$ b [23]. At present, we have calculated the second term with $\delta_L\mathcal{F}$ from Eq. (6) and found that it gives approximately 1% as compared with the first term. Though the contribution of the terms with $\delta_L\mathcal{F}$ and $\delta_L\mathcal{F}^\xi$ in non-magic nuclei should be analyzed specially, it can hardly be considerable in the problem under consideration and is omitted in the present calculations.

We calculated the quadrupole moments of the first $2^+$ states in non-magic tin and lead isotopes according to Eqs. (8 – 10) in the $\lambda$-representation with self-consistent single-particle wave functions $\phi_\lambda$ obtained within the EDF method [13] with the functional DF3-a [14]. The spherical box of the radius $R$=16 fm was used to simulate the single-particle continuum. We examined the dependence of calculation results on the cut-off energy $E_{\rm max}$ and have found that the value of $E_{\rm max}$=100 MeV

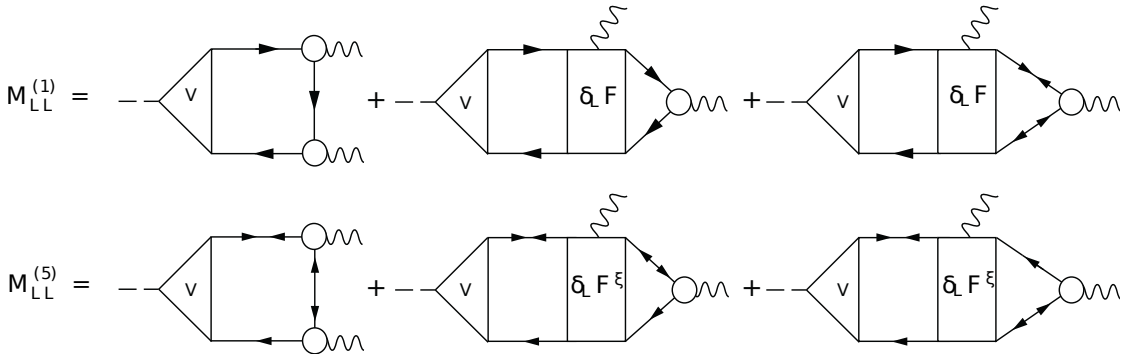


FIG. 4: Matrix elements for $M^{(1)}_{LL}$ and $M^{(5)}_{LL}$ for non-magic nuclei.

ensures 1% accuracy. To calculate the quantities V and $g_L$, the results of our previous article [20] have been used where all the calculations were performed in the coordinate representation using the same self-consistent DF3-a basis as in the present calculation of the matrix element $M_{LL}$. Thus, no fitted parameters was used in the present calculations.

The results are given in Table 1 and Figs. 1, 2. Except for the case of $^{112}$Sn and $^{208}$Pb nuclei, we obtained a reasonable agreement with experimental data [23]. Unfortunately, they have rather big errors so that we need some better measurements to check our approach.

We have also calculated the contribution of the ground state correlations term in Eq. (9) (see the discussion at the end of Sect. III) and obtained that it is rather considerable. For some nuclei it is about 60% of all the triangle contribution. This very interesting result will be discussed in more detail separately.

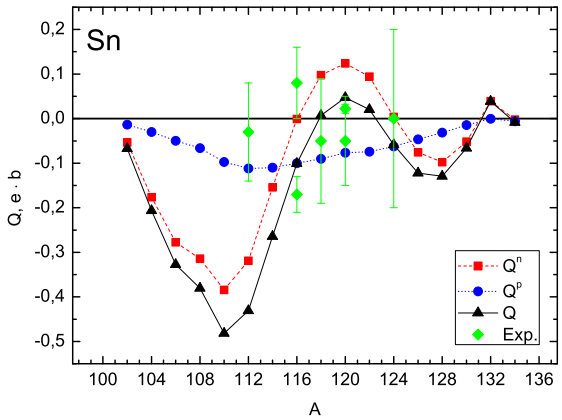


FIG. 5: (Color online) Quadrupole moments of the first 2+ excited states in even Sn isotopes.

TABLE I: Quadrupole moments $Q$ (e b) of the first $2^+$ states in Sn and Pb isotopes. ($Q^n$ and $Q^p$ are the neutron and proton contributions to the final result $Q_{\rm tot}$=$Q^n$ + $Q^p$. )

| nucl. | $Q^{\rm n}$ | $Q^{\rm p}$ | $Q_{\rm tot}$ | $Q_{\rm exp}$ [23] |
|---|---|---|---|---|
| $^{102}$Sn | -0.05 | -0.01 | -0.07 | – |
| $^{104}$Sn | -0.18 | -0.03 | -0.21 | – |
| $^{106}$Sn | -0.28 | -0.05 | -0.33 | – |
| $^{108}$Sn | -0.31 | -0.07 | -0.38 | – |
| $^{110}$Sn | -0.38 | -0.10 | -0.48 | – |
| $^{112}$Sn | -0.32 | -0.11 | -0.43 | -0.03(11) |
| $^{114}$Sn | -0.15 | -0.11 | -0.26 | 0.32(3), 0.36(4) |
| $^{116}$Sn | 0.00 | -0.10 | -0.10 | -0.17(4), +0.08(8) |
| $^{118}$Sn | 0.10 | -0.09 | 0.01 | -0.05(14) |
| $^{120}$Sn | 0.12 | -0.08 | 0.05 | +0.022(10), -0.05(10) |
| $^{122}$Sn | 0.09 | -0.07 | 0.02 | -0.28 < $Q$ <+0.14 |
| $^{124}$Sn | 0.00 | -0.06 | -0.06 | 0.0(2) |
| $^{126}$Sn | -0.08 | -0.05 | -0.12 | – |
| $^{128}$Sn | -0.10 | -0.03 | -0.13 | – |
| $^{130}$Sn | -0.05 | -0.01 | -0.07 | – |
| $^{132}$Sn | 0.04 | 0.00 | 0.04 | – |
| $^{134}$Sn | 0.00 | -0.01 | -0.01 | – |
| $^{190}$Pb | -0.60 | -0.29 | -0.89 | – |
| $^{192}$Pb | -0.77 | -0.35 | -1.12 | – |
| $^{194}$Pb | -0.90 | -0.39 | -1.28 | – |
| $^{196}$Pb | -0.85 | -0.38 | -1.23 | – |
| $^{198}$Pb | -0.67 | -0.35 | -1.02 | – |
| $^{200}$Pb | -0.27 | -0.23 | -0.50 | – |
| $^{202}$Pb | 0.02 | -0.15 | -0.13 | – |
| $^{204}$Pb | 0.18 | -0.07 | 0.11 | +0.23(9) |
| $^{206}$Pb | 0.11 | -0.02 | 0.10 | +0.05(9) |
| $^{208}$Pb | 0.01 | 0.04 | 0.05 | -0.7(3) |

## V. CONCLUSION

We have considered the method to calculate static moments of the excited states and transitions between excited states, which, generally speaking, are described within the QRPA, with taking all the $g^2$ terms into account in magic and non magic nuclei. It was shown that, in addition to the old results [17, 19], new terms with

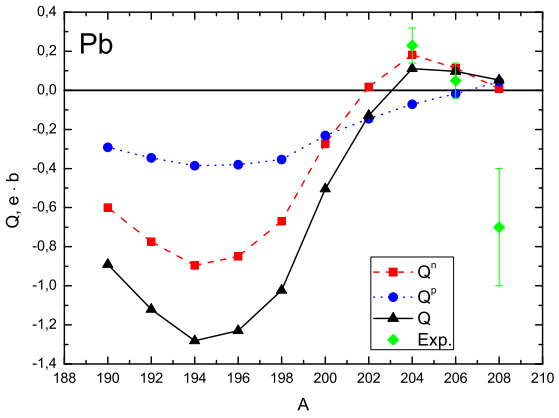


FIG. 6: (Color online) Same as in Fig.5 but for Pb isotopes

$\delta_L F$ and $\delta_L F^\xi$ appear, which contain the density dependence of both the ph and pp effective interactions. We have performed the self-consistent calculations of the static quadrupole moments of the first $2^+$ states for Sn and Pb isotopes using the known functional's parameters set DF3-a. Except for the $^{112}$Sn and $^{208}$Pb cases, a reasonable agreement has been obtained with the experiment available, though, as a rule, the experimental data have big errors. In these calculations we did not take into account new terms with $\delta_L F$ and $\delta_L F^\xi$ . As all modern microscopic calculations deal with the density dependence of ph and pp effective interactions, it is important to analyze their role in the problems under consideration. This rather complicated problem will be considered separately.

## VI. ACKNOWLEDGMENT

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